

Statistics of Deep Energy States in Coulomb Glasses

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We study the statistics of local energy minima in the configuration space and the energy relaxation due to activated hopping in a system of interacting electrons in a random environment. The distribution of the local minima is exponential, which is in agreement with extreme value statistics considerations. The relaxation of the system energy shows logarithmic time dependence reflecting the *ultrametric* structure of the system.

Possible phases and the corresponding dynamic behaviors of strongly correlated disordered systems remain one of the central unresolved issues. Doped semiconductors in the insulating state are an exemplary system endowed with strong long-range Coulomb interactions and strong disorder. It was hypothesized that the combined action of both inflict the glassy phase, resulting in the term *electron- or Coulomb glass* [1]. Ever since, a Coulomb glass has been a subject of the intense research, see [2]; however, despite the impressive developments, a consistent picture of its nature is still not available and the consensus on the interrelation between its inherent glassy ingredients like Coulomb gap, slow dynamics and aging, the nature of the low-lying metastable states and the mechanisms of hopping transport is not yet achieved. A classic qualitative derivation [3] of the Coulomb gap induced in the single-particle density of states due to pair correlations remains the top result in the field.

One of the main characteristics of the glassy state is the existence of an infinite number of low-lying states (valleys in the rugged free energy relief) separated by barriers growing infinitely in the thermodynamic limit. This picture emerged from the study of the infinite range interaction model for spin glasses (Sherrington-Kirkpatrick spin glass) [4] and was later shown to imply *an ultrametric structure* of the configurational space [5].

There was important recent progress in relating the appearance of the Coulomb gap in electron systems to the generic glassy behavior [6], where a lattice model of spinless interacting electrons in the presence of randomness was considered and a nonlinear screening theory was formulated to tackle Coulomb gap formation and its relation to glassy freezing. The formation of the glass phase with a large number of metastable states was identified via the emergence of a replica symmetry breaking instability. In [7], the connection between the glass phase characteristics and a Coulomb gap was argued, noticing that within the locator-approximation the correlated electron system maps to the Sherrington-Kirkpatrick spin glass. Remarkably, recent experimental studies of low-frequency resistance noise in silicon inversion layers indicated glassy freezing and the presence of long-range

correlations, consistent with the hierarchical picture of glassy dynamics [8]. This gives strong support to a hierarchical structure of experimentally observed Coulomb glasses and calls for further comprehensive study of hierarchical glassy systems.

In this Letter we demonstrate that the distribution of low-lying energy states in systems with an ultrametric configurational space obeys *extreme value statistics* giving rise to an exponential distribution for the extremely low energies, $p \propto \exp(-E/E_0)$, where E_0 is a characteristic energy. The exponential tail is verified numerically for the lattice model of a disordered Coulomb system. We find that system's energy relaxes with time following the $\log t$ law, as indeed expected for ultrametric hierarchical structures [9]. This offers strong evidence that electronic systems with long-range Coulomb interactions form a Coulomb glass with exponential distribution of lowest energy states.

Exponential distribution.— We start with the derivation of the exponential statistics for the low-lying energy states of systems with ultrametric topology of the configurational space. This space can be represented graphically as a hierarchical tree which is the union (or sum) of hierarchical trees with branching numbers $n \in \mathbb{N} \setminus \{1\}$ (n -trees, see Fig. 1). The crown of the tree (leaves) corresponds to a set of nearly equal energies that form an almost degenerate ground state of the system. We consider now the subset of the configurational space characterized by an n -tree and find the distribution function of

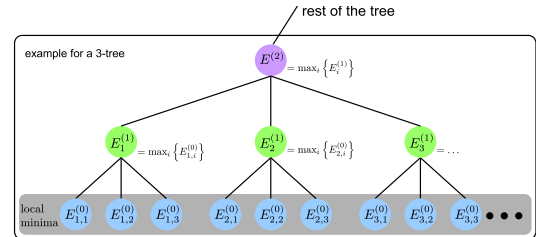


FIG. 1: Illustration of a 3-tree, an element of the hierarchical tree representing the configurational space with ultrametric topology.

the corresponding lowest energy states. It is convenient to introduce positive variables $\{E\}$ measuring the *depths* of the potential wells. Starting with the lowest hierarchical level (crown) consider one of the sibling states sets, $\{E_i^{(0)}; i \in \mathbb{N}^{\leq n}\}$, where the superscript (0) marks the lowest hierarchy level. We define $E_1^{(1)} \equiv \max_{1 \leq i \leq n} \{E_i^{(0)}\}$ and assign it to the branching point level (1) generating the considered 0-th set of siblings. Now we have a collection of level-(1) sibling n -sets. Repeating the procedure, we obtain the next generation of low-lying energies $\{E_i^{(2)}\}$ that constitute the assortment of the second level sibling n -sets. The described iteration should converge to a limiting distribution for the probability $\mathcal{P}_n(E^{(j)})$ for the lowest states at the j -level of the hierarchy, as $j \rightarrow \infty$. This distribution must be stable under the max operation. In other words if $E \equiv \max_i \{E_i\}$ then the probability distribution of the extrema E is the same as that of each member E_i of the set. The distribution we seek belongs to the class of so-called extreme statistics [10].

To briefly summarize the theory of extreme distributions, we consider a set of identically distributed independent random variables X_i , with $1 \leq i \leq n$ (in the present problem these are all the low-lying energies within one set of sibling states). Let $M_n = \max_{1 \leq i \leq n} \{X_i\}$ and let $\mathcal{P}_1(x)$ be the probability that any of the random variables X_i is less than x . The probability that the largest value, M_n , of the set $\{X_i; i \in \mathbb{N}^{\leq n}\}$ is less than x is simply the probability that all of the X_i 's fall short of x . Since the variables are independent, this is given by

$$\mathcal{P}\left(\max_{1 \leq i \leq n} \{X_i\} \leq x\right) \equiv \mathcal{P}_n(x) = [\mathcal{P}_1(x)]^n. \quad (1)$$

The central concept of the theory of extreme statistics is the *stability postulate* [10], stating that after many iterations the distribution describing M_n for a sufficiently large set $\{X_i\}$ is the same as the distribution for each variable X_i . This requires that the probability $\mathcal{P}_n(x)$ satisfied the functional equation $\mathcal{P}_n(x) = [\mathcal{P}_n(a_n x + b_n)]^n$, where a_n and b_n are positive constants. It can be shown that, under rather nonrestrictive assumptions about the initial distribution of random variables $\{X_i\}$ there are only three classes of distribution functions depending on its support. In particular, if $x \in \mathbb{R}$,

$$\mathcal{P}_n(x) = \exp[-n \exp(-x)], \quad a_n = 1, \quad b_n = \ln(n), \quad (2)$$

and, therefore, the limiting form for a distribution of the lowest energy states corresponding to an n -tree subset of the configurational space is $\mathcal{P}_n(E) = \exp[-n \exp(-E)]$, where E is measured in dimensionless energy units.

As mentioned before, the configurational space of our system endows with an ultrametric structure which can be represented as an union of all possible n -trees. Therefore the global *distribution density* can be found as

$$p(E) = \int dn w(n) \frac{d\mathcal{P}_n(E)}{dE}, \quad (3)$$

where $w(n)$ is the weight of the n -trees in the configurational space. The weight $w(n)$ is determined by the physical properties of the system in question. In our case one observes that the elemental process of generating two nearly degenerate energy states is the pair electron exchange within a specially arranged compact 4-sites aggregate [11]. Analogously, compact aggregates allowing the exchange of n pairs, generate the same number of sibling states of the corresponding hierarchical trees. Thus $w(n)$ is nothing but the percolation cluster size-distribution function: $w_n \propto n^{-s}$, where $s \geq 2$. Plugging this weight into Eq. (3) one arrives at the exponential density distribution for the low-lying energies, $p(E) \propto \exp(-E/E_0)$, where s is absorbed into the normalization energy E_0 .

The extreme value distributions for extremely low-energy states belongs to the so-called were derived [12] for several systems and problems possessing one step replica symmetry breaking solutions, such as the random energy model and decaying Burgers turbulence. It was found that extremely low energy states of elastic manifolds in random environment (modeling a rich variety of physical systems including vortices in superconductors, charge density waves, Wigner crystals, domain walls, and many others) also obey exponential statistics resulting in creep motion which is specific for glassy states [13]. Our results taken together with those of [12, 13] allow to arrive at the conclusion that the exponential distribution of the extremely low-lying energy states, the resulting creep response, and the related $1/f$ noise [14] are generic properties of all strongly correlated disordered systems possessing a fractal structure of configurational space.

Model.— Now we turn to numerical studies of the energy configurational space. The lattice Coulomb model was studied numerically in the past [15, 16, 17], the typical system size was about 10^2 . Optimized numerical procedures enabled us to consider 100-times larger systems and analyze about 10^5 different energy minima. The Hamiltonian of a 2D Coulomb lattice with disorder

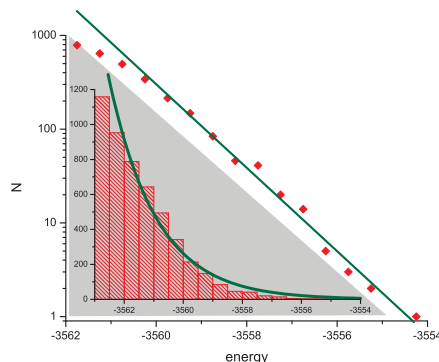


FIG. 2: Energy distribution of about 12000 local minimum states in half-log representation with linear fit. Linear scale with exponential fit (triangular inset).

is

$$\mathcal{H} = \sum_i \varepsilon_i, \quad \varepsilon_i = U\alpha_i n_i + \frac{e^2}{2} \sum_{j \neq i} \frac{(n_i - \nu)(n_j - \nu)}{r_{ij}}, \quad (4)$$

where i and j label the lattice sites, $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, $U\alpha_i$ with $\alpha_i \in [-1; 1]$ define the quenched uniformly distributed random site energies, and n_i are the occupation numbers (values 0 or 1) with average ν .

The simulations were performed on the lattices with typically $N = 100^2$ sites with periodic boundary conditions and the filling factor $\nu = 0.5$. We took the disorder spread, U , be equal to the Coulomb interaction at the distance of the lattice constant. Consequently, U , the lattice constant, and e were set to unity; vectors \mathbf{r}_i label square lattice sites. The behavior of the system is governed by the interplay between disorder and Coulomb interactions. At very weak disorder the system is crystal-like; increase in U brings glassy behavior.

Local minima.— To track down local minima of the system free energy, we choose an arbitrary initial distribution of electrons and perform sequential transfer of electrons between the adjacent sites (of course such an elemental hop can be realized only if the target neighboring site is vacant). At each step the total Coulomb energy of the system is calculated using Eq.(4). If any nearest site hop gives rise to the increase in total energy, as compared to its value at previous step, the state and the corresponding energy is marked as energy minimum. In subsequent iterations one finds transfers that decrease total energy executing thus dissipation of the system into more and more deep energy valleys. Note that this algorithm lists *all* the possible low-lying states. To ensure evolving the system into true low lying minima we were starting collection statistics after reaching the states where at least 10^5 random hops were needed to go from one local minimum to another. Shown in Fig. 2 is the obtained distribution of energies corresponding to local minima; one sees that the distribution tail obeys the exponential law, $N_{\min}(E) \sim e^{-E/E_0}$.

For all the computed minima we define the normalized site occupation number difference $\Delta_{\alpha\beta} = N^{-1} \sum_i |n_i^\alpha - n_i^\beta|$ corresponding to all pairs of minima $\{\alpha, \beta\}$. The distribution of $\Delta_{\alpha\beta}$, i. e., the fraction of the system which has different occupation numbers for two different minima is shown in Fig. 3. To drive our system (the filling factor 0.5) from one minimum to another, about 5.4% of the electrons has to be transferred to different lattice sites. This shows that the (pseudo-)ground state of our system is indeed highly degenerate: it is enough to move around only a few electrons in order to get into another energetically close local minimum. This well illustrates the ultrametric structure of the configurational space.

The $\Delta_{\alpha\beta}$ distribution is also calculated for smaller systems with the same filling factor. For system sizes above $\approx 25^2$ the fraction of the electrons different between min-

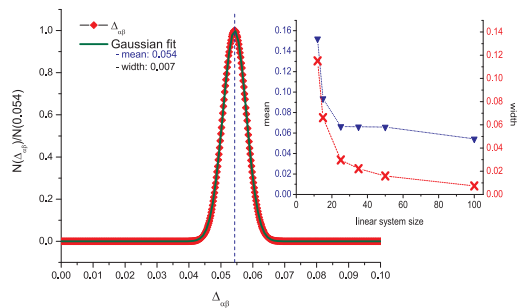


FIG. 3: Distribution of the difference of the local minima $\Delta_{\alpha\beta}$ (0 for identical states, 1 for complementary ones). The distribution is fitted by a Gaussian curve, with mean at 0.054 and width 0.007. 10^7 overlap integrals are calculated. The inset shows the dependence of the mean and width of the distribution on system size.

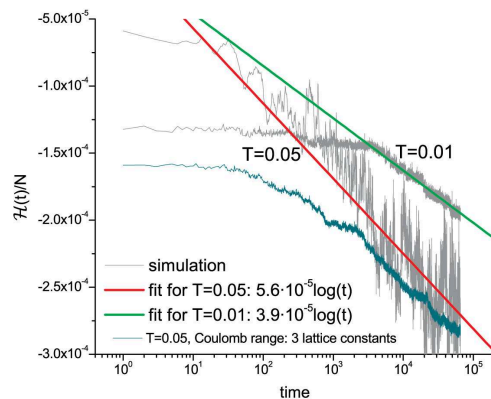


FIG. 4: Energy relaxation of the system energy for two different temperatures. In the two upper plots logarithmic fits are shown. At lower temperatures ($T = 0.01$) the initial “flat” region is due to a very long equilibration phase of the system to reach the steady state from the local minimum. Even after averaging over several time series the fluctuations at higher temperatures are still large. At even higher temperatures the fluctuations dominate and the logarithmic behavior cannot be recognized since due to computational limits no more averaging can be done in reasonable time. The lower graph shows the energy relaxation for the case when the Coulomb interaction range is artificially limited to 3 lattice sites at $T = 0.05$. One sees (1) that the behavior deviates from the log behavior and (2) the amplitude of the fluctuations are much smaller as for the case with full Coulomb interaction.

ima and the width of the distribution stay essentially the same. Both increase upon lowering the system size; see inset in Fig. 3. For very small systems (below 15^2) the distribution is not Gaussian anymore since there is only a small number of possible local minima. This indicates that small systems do not have an ultrametric structure and therefore do not represent physical systems.

Energy relaxation.— Next we analyze the relaxation of the system at finite temperatures. Due to the ultrametric structure of the system the relaxation can be described as diffusion or random walk on the tree representing the structure [9] (Fig. 1). Starting from a local

minimum, nearest neighbor hopping with Boltzmann factors $e^{-\Delta\varepsilon_{ij}/T}$ is applied to all particles in the system - random permutations are used to address the lattice positions in one time step. The typical energy difference $\Delta\varepsilon_{ij}$ of two adjacent lattice sites i and j is of order one in the used dimensionless units.

In Fig. 4 the time evolution of the system energy is shown for two different low temperatures. Since the relaxation is very slow and the fluctuations are significant (even after averaging over several time series) and furthermore increase with temperature, a conclusive discrimination of the behavior is not possible. However, it can be well fitted by a logarithmic law in agreement with the result of [9]. This lends an additional support to the hypothesis of the glassy nature of long-range interacting, disordered Coulomb systems. Previously the time evolution in the Coulomb lattice model was studied via Monte-Carlo methods, see e.g. [18, 19, 20]. In [20] the energy relaxation observed via evolution of the system after adding a few electrons showed $1/t$ -behavior.

Finally, we investigated the relation between the relaxation of the system and electron correlations reducing artificially the screening length of the Coulomb interaction (in all other simulations the range is of order of the system size). In this case the relaxation deviates from the $\log t$ law (see lower curve in Fig. 4) indicating the crucial role of long-range interactions in forming Coulomb glass.

Discussion and conclusions.— In conclusion, we have derived that in a system endowed with an ultrametric configurational space the local energy minima follow extreme value statistics resulting in an exponential distribution of the low-lying energy states. Since in the most strongly correlated disordered systems the energy landscape is expected to be characterized by only one energy parameter, one can assume that barriers separating the low-lying states also obey the same statistics. This suggests that the nonlinear creep dynamic response and the related $1/f$ noise are generic properties of all strongly correlated disordered systems.

Our numerical results for a disordered system with long-range Coulomb interaction – including the exponential distribution of the low-lying energy states and the logarithmic time relaxation of the system towards its ground state – offer strong evidence towards the existence of a Coulomb or electronic glass and relates the formation of the glassiness with long-range correlations in Coulomb systems. This further explains why pronounced glassy properties like aging and memory effects as well as apparently unbounded $1/f$ noise are observed in electronic systems with profound long-range electron-electron interactions. Of course the specific manifestation of the energy statistics in the observable quantities requires concrete consideration of the peculiarities of the physical system

involved and goes beyond the scope of this work. In particular, one of the most intriguing questions concerning the behavior and the nature of the noise in various disordered electronic systems will be the subject of a forthcoming publication.

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